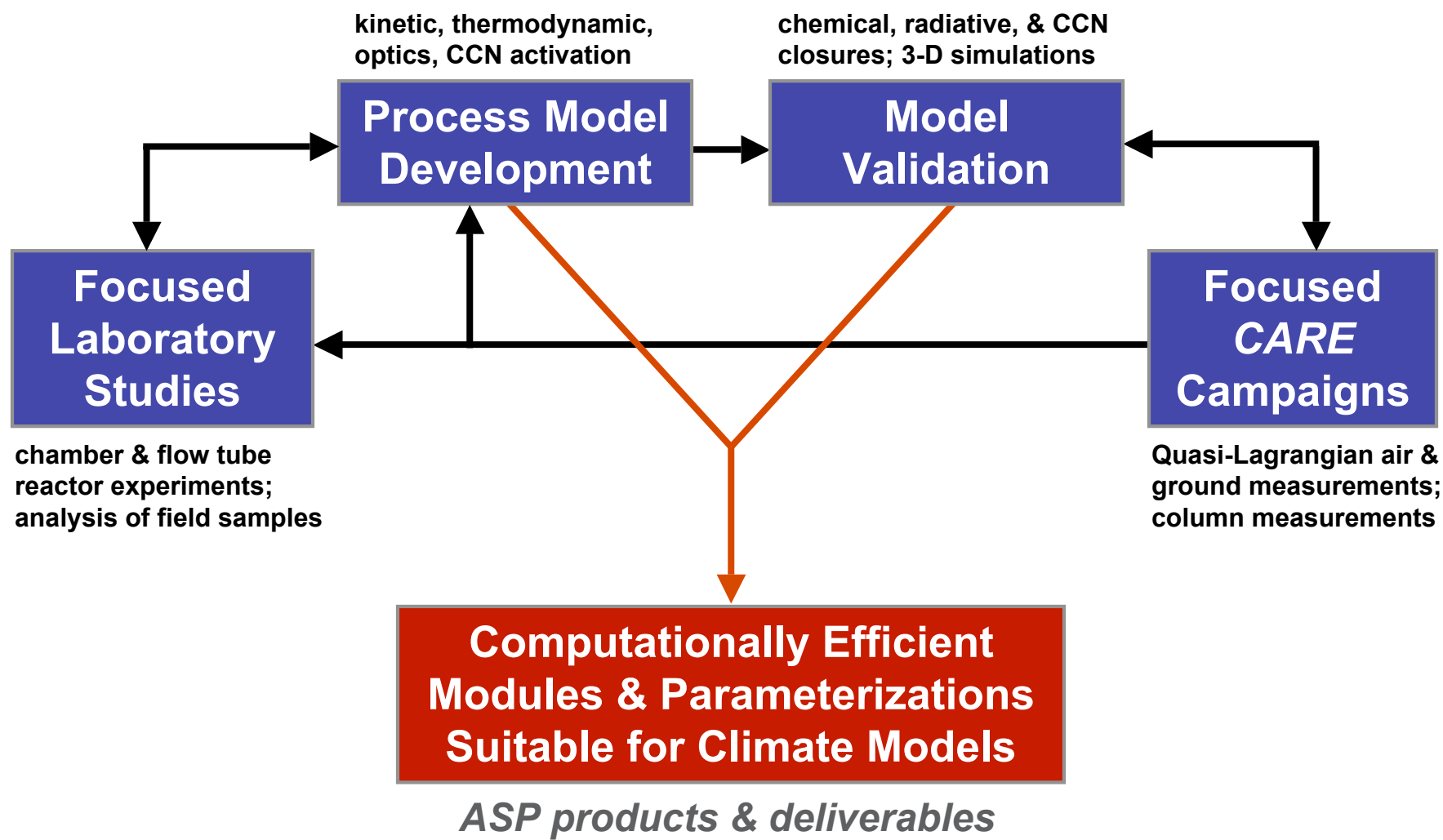


Gas-Particle Interactions Working Group

Summary

DOE ASP Meeting
Boulder 26-Oct-2006
Rahul Zaveri, Chair

Integrated lab-model-field components...



Future Field Campaign Discussion

- S. Madronich: SOA formation is ridiculously poorly understood. Global models have to incorporate the much higher SOA observed.
- S. Schwartz: use “5x” in FORTRAN is not the solution we want.
 - R. Zaveri: We don’t know if “5x” holds for long field evolution.
 - S. Madronich: Cannot capture future evolution in anthropogenic emissions from developing countries, or due to land use changes. So cannot predict the consequences of human activities, so cannot inform policy.

Field Campaigns

- J. de Gouw: many years till we understand the problem from first principles. Maybe some value in using parameterizations (arising from field work) inside the models.
- D. Worsnop: MILAGRO workshop shows that we need to design field experiments that have the appropriate combinations of biogenic, anthropogenics, and biomass burning emissions. Span the range of chemistries and conditions.

Field Campaign

- Maybe focus on biogenics – most uncertain
- Get closure on biogenic SOA
- Go back to urban-biogenic in US/Canada
- Start planning another MILAGRO/GVAX now (5-6 years lead time)

Model Development

- New Process Models
 - Revisit model framework
 - Is partitioning theory working?
 - Test against lab studies

Laboratory Studies

- Need to design better laboratory studies
 - Time scales in a smog chamber relevant to initial SOA formation observed in urban areas
 - Studies should focus on urban VOCs and interactions between urban and biogenic VOCs
 - Focus on heterogeneous chemistry
 - Develop new models that can reliably explain the urban SOA field observations

Sasha Madronich

- Working on self-generating mechanism for organic reactions. Generates 10^5 reactions by 10^4 species.
- Working, in the last year have updated aromatics using Leeds Master Mechanism. Can now handle cyclic compounds, which had technical difficulties. Can now calculate Henry's law coefficients and vapor pressures.
- Want to apply to Mexico City to predict organic photochemistry and SOA.

Yin-Nan Lee

- Two experiments since last meeting, MASE and MAX-MEX.
- All data is in place for MASE, and taking a closer look at it now. Did NOT see a strong effect of organics on activation of particles near stratus clouds. Just got the AMS data and will be looking at size-resolved composition
- MILAGRO, good dataset to evaluate models of gas-particle partitioning

Mary Gilles & Alex Laskin

- Looking at BC characterization
- MILAGRO looks beyond ideal from the first look at the data. BC has some organics even at T0. Lots of work to do.
- Studied Tar-balls, looks more like HULIS
- Participated in MASE, was good to work with Alex, he can screen through 10^4 particles, can find particles for Mary to look at.

Luisa Molina

- Continue to analyze data from MCMA-2003. E.g. Volkamer et al. SOA study. Also posters on O₃ formation.
- Participated in MILAGRO. DOE support is for continuing the 2003 work, using DOAS. Long path does and also a network of MAX-DOAS around MCMA.
- Also working with Alex Laskin and Mary Gilles & Aerodyne and Colorado
- Also working with Spyros Pandis to develop PMCAMx particle model. Hopefully ready by the end of the year.

Jay Slowik

- Developed system to characterize soot shape, size and morphology.
- Carried out intercomparison study of different techniques, interesting results on the effect of coatings.
- Did experiment at T0 during MILAGRO, saw increases in particle mass and changes in shape (fractal -> spherical) due to coating with secondary aerosols. Seen nice correlations with data from A Laskin and M Gilles. More work to do.
- Want to work with modelers

Mike Ezrell / B Finlayson-Pitts

- Looking at NaNO_3 particles in the wall of a chamber, with gas-phase α -pinene. When photolyzing with black-lights see new particle formation and growth.
- Have collaborated with A. Zelenyuk at PNNL. See organic in particles, decrease in density.
- Now down to 1 ppm, will go to 0.1 ppm soon. Also several other experiments, including flowtube.

Albert Chung / S. Paulson

- Built outdoor photochemical chamber at roof in UCLA. Generated aerosols with diesel generator, conventional diesel and biodiesel. Also toluene.
- Using polar nephelometer, measures refractive index of aerosols (discussed earlier in prez). Hope to measure at ambient concentrations. Hope to measure both real and imaginary parts of refractive index (haven't tested imaginary yet).

Doug Worsnop

- Continued to work in MCMA-2003 dataset. Both in emissions (chase and traffic sampling) and data from three sites that is being put in a photochemical context for MC.
- Deployed mobile lab again during MILAGRO. Have data from Pico Tres Padres, Tula, and other sites. Want to model sources and receptors of emissions and SOA.
- Supported soot evolution study with BC and other groups.
- Have Pb observations at three sites. Trajectories indicate most of it coming from Tula. SOA/CO ratios that indicate SOA increases with photochemical age.
- Gas-phase NH_3 and particle NO_3 particles, want to analyze partitioning of NH_4NO_3 . See anticorrelation of nitric acid and nitrate.
- See new particle formation events at Tres Padres.
- Using AMS and PTR-MS, looking for tracers of biomass burning.
- Want to integrate with other sites and models.

Steve Springston

- Participated in MASE and MAX-MEX over the last cycle.
- Produced data merges of those datasets and made them available.
- Lots of effort on data validation, comparing G-1 measurements with ground sites and other aircraft.
- Particle absorbance/CO clearly increasing downwind of Mexico City.

John Jayne - ARI

- Through DOE SBIR program, supported an aircraft version of the C-ToF-AMS. It flew successfully during MAX-MEX.
- Data submitted, working with Steve in merging it together, to make it accessible to modelers.

Liz Alexander

- Building PTR-ion trap MS. Expanded because now have access to high-resolution ToF. Interchangeable with linear quadrupole and ion trap. Will start testing that in a couple of months.
- Ion trap should be able to resolve isobaric interferences. Others have found lower sensitivity than desired. But interface in this project is different, it should be much more sensitive.
- W-ToF can resolve isobaric interferences either with the high resolution, or with MS/MS with SID.
- It will provide higher sensitivity and time resolution. Ion trap and W-ToF also give full spectrum rather than a subset of m/z . Also helps to distinguish some of the interferences between VOCs.
- Not ASP-funded but related: new particle collectors, then heat to desorb semivolatiles.

Rahul Zaveri

- Working on modeling. MOSAIC. Model for simulating aerosol interactions and chemistry.
- Simulates many processes.
- Published two papers, third will be submitted soon.
- Hoping to work over the coming year on integrating SOA formation into MOSAIC. Also interested in collaborating with other people who have measurements that can be integrated or compared with models.

Jose-Luis Jimenez

- Working on analysis of MCMA-2003 field campaign, collaborating with Aerodyne and Molina. Published papers on larger than expected SOA formation w/ Rainer, and on characterization of aerosols during the campaign. Another two papers are submitted and should be published in a few months (on PAHs and particle shape). Very exciting results on component analysis of AMS spectra, can estimate separate contributions of POA, SOA, and biomass burning in Mexico City.
- Large effort in MILAGRO field campaign. Deployed high-resolution AMS to T0 site, and also a thermal denuder, an SMPS, nano-SMPS, and aerosol concentrator. Also deployed a Q-AMS for flux measurements at RAMA site. All very successful, now doing data analysis.
- Preliminary analysis of MILAGRO: high fraction of oxygenated organics, ~5% organic fragments (some amines). Also urban POA is more volatile than oxygenated organics (SOA), which is the opposite of how they are represented in models.